Path Homology Theory of Digraphs and Its Applications to Brain Network Analysis

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Presentation Summary

Introduction

Why go beyond Graph Theoretical Analysis?

Graph theory is based on an overly simplistic premise: two nodes (neurons or brain regions) connected by an edge. "Dyadic relationships fail to accurately capture the rich nature of the system's organization" (Giusti et al., 2016).

Usual graph measures, such as clustering coefficient, may sometimes not properly capture the topology of the network. For instance, given two nodes with the same clustering coefficient, the topology of their neighbourhoods can be significantly different (Kartun-Giles et al., 2019).

Network topology has been shown to be an important tool for analyse network structure, and generalizations of graphs such as simplicial complexes and path complexes may overcome these limitations.

Our Primary Motivation: Brain Connectivity Networks

Most of the graph theoretical analysis (GTA) methods used in network neuroscience are for undirected graphs (recently extended to undirected simplicial complexes), and since we are estimating brain networks via information partial directed coherence (iPDC) (Takahashi et al., 2010a; Takahashi et al., 2010b), we should develop a good framework for working with directed graphs and directed simplicial complexes.

The most general approach (which generalizes directed simplicial complexes) is a new formalism proposed in a series of articles between 2013 and 2015 by Grigor'yan et al. (Grigor'yan et al., 2014a; Grigor'yan et al., 2014b; Grigor'yan et al. 2015a; Grigor'yan et al., 2015b) called path complexes.

Why Path Complexes and Path Homology?

Given a digraph, we can use the simplicial homology as a topological descriptor by obtaining a simplicial complex from the clique complex (or flag complex) of the underlying undirected graph, which implies discarding the directionality.

However, we can use the path complex associated with the digraph, which preserves directionality and contains additional structures beyond the cliques.

For instance, a directed square $a \to b \to d$, $a \to c \to d$ has no triangles, yet it is taken into account in the calculation of the path homology, as we will see in the next slides. For this structure, we have two parallel routes from a to d, and simplicial/flag homology cannot see this, but path homology can.

The Theory of Path Complexes and Path Homologies

Paths in a Finite Set

Let V be a finite set. For any $p \geq 0$ an elementary p-path is any sequence of $p+1$ vertices of V that will be denoted $e_{i_0 \dots i_p}$. A p-path over a field $\mathbb{K}$ is any formal $\mathbb{K}$-linear combinations of elementary p-paths, that is, any p-path has a form

$$u = \sum u^{i_0 \cdots i_p} e_{i_0 \dots i_p}. \tag{1}$$

where $u^{i_0 \cdots i_p} \in \mathbb{K}$. We denote by Λ_p the $\mathbb{K}$-linear space of all p-paths. For example, $\Lambda_0 = \mathrm{Span}\{e_i : i \in V\}$, $\Lambda_1 = \mathrm{Span}\{e_{ij} : i, j \in V\}$, $\Lambda_2 = \mathrm{Span}\{e_{ijk} : i, j, k \in V\}$.

Definition: A path $i_0 \cdots i_p$ is *regular* if $i_k \neq i_{k+1}$ for all k, and *irregular* otherwise (some *consecutive* repeat).

The Boundary Operator and Paths in a Digraph

Definition: For any $p \geq 1$, we define the p-th boundary operator $\partial_p : \Lambda_p \to \Lambda_{p-1}$ by

$$\partial_p e_{i_0 \dots i_p} = \sum_{q=0}^{p} (-1)^q e_{i_0 \dots \hat{i_q} \dots i_p}. \tag{2}$$

For instance, $\partial_1 e_{01} = e_1 - e_0$ and $\partial_2 e_{012} = e_{12} - e_{02} + e_{01}$.

Definition: Let $G = (V, E)$ be a digraph. An elementary p-path $i_0 \dots i_p$ on V is called allowed if $i_k \to i_{k+1}$ for any $k = 0, .., p-1$ and non-allowed otherwise.
Let $\mathcal{A}_p$ the $\mathbb{K}$-linear space spanned by allowed elementary p-paths:

$$\mathcal{A}_p = \mathrm{Span}\{e_{i_0 \dots i_p} : i_0 \dots i_p \text{ is allowed}\}. \tag{3}$$

∂-Invariant Paths

Consider the following subspace of $\mathcal{A}_p$:

$$\Omega_p = \Omega_p(G) := \{u \in \mathcal{A}_p : \partial u \in \mathcal{A}_{p-1}\}. \tag{4}$$

Definition: The elements of Ω_p are called ∂-invariant p-paths.

Hence, we obtain a chain complex of ∂-invariant paths, $\Omega_\bullet = \Omega_\bullet(G)$:

$$0 \leftarrow \Omega_0 \xleftarrow{\partial} \Omega_1 \xleftarrow{\partial} \dots \xleftarrow{\partial} \Omega_{p-1} \xleftarrow{\partial} \Omega_p \xleftarrow{\partial} \dots$$

Example: A directed triangle is a sequence of three vertices a, b, c such that $a \to b \to c$, $a \to c$. A directed triangle determines a 2-path $e_{abc} \in \Omega_2$ because $e_{abc} \in \mathcal{A}_2$ and $\partial e_{abc} = e_{bc} - e_{ac} + e_{ab} \in \mathcal{A}_1$.

Path Complexes

Definition: A path complex over a set V is a non-empty collection $\mathfrak{P}$ of (regular) elementary paths on V with the following property:

- for any $n \geq 0$, if $i_0 \dots i_n \in \mathfrak{P}$ then also the truncated paths $i_0 \dots i_{n-1}$ and $i_1 \dots i_n$ belong to $\mathfrak{P}$.

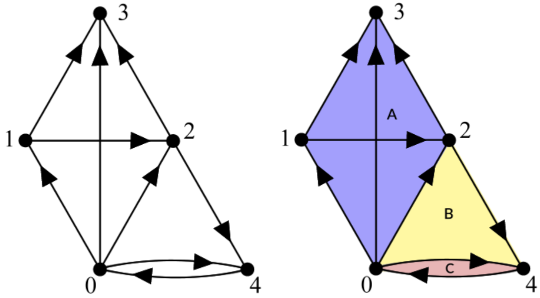
Definition: Given a *digraph* $G = (V, E)$, $E \subseteq \{(i, j) : i \neq j\}$ (no loops), its path complex $\mathfrak{P}(G)$ consists of all regular paths $i_0 \cdots i_p$ that are *walks*: $(i_{k-1}, i_k) \in E$ for every k.

Note that deleting the first or last vertex of a walk is still a walk, so $\mathfrak{P}(G)$ is a path complex. Hence every digraph has a path homology.

Also, note that path complexes generalizes the notion of directed clique complexes, since every directed p-clique can be identify as a ∂-invariant p-path $e_{i_0 \dots i_p} \in \Omega_p$.

Example of Path Complex associated with a Digraph

Allowed p-paths: $e_{04}, e_{040}, e_{024}, e_{013}, e_{0124}$, etc.;
Directed cliques: A: $\{e_{0123}, e_{03}, e_{12}, e_{13}\}$ (directed 3-clique); B: $\{e_{024}, e_{04}\}$ (directed 2-clique);
Double edge: C: $\{e_{040}\}$.



Note that e_{0123} can be identified as the directed 3-clique A, since e_{0123} is ∂-invariant. Similarly, e_{024} can be identified as the directed 2-clique B.

Path Homologies

Given a digraph G, the path homology its path complex $\mathfrak{P}(G)$ is the homology of $(\Omega_\bullet, \partial)$:

$$H_p(G) = H_p(\mathfrak{P}(G)) = \frac{\ker \partial\big|_{\Omega_p}}{\operatorname{Im} \partial\big|_{\Omega_{p+1}}}.$$

Betti numbers: $\beta_p(G) = \dim H_p(G)$. Euler characteristic:

$$\chi(G) = \sum_{p=0}^{\infty} (-1)^p \beta_p(G) = \sum_{p=0}^{\infty} (-1)^p \dim \Omega_p(G).$$

Examples: Path Homologies of a Single Arc and a Directed Triangle

Example 1. Let G consist of two vertices $\{0, 1\}$ and a single arc $0 \to 1$. Then $\Omega_0 = \mathbb{Z}^2$, $\Omega_1 = \mathbb{Z}\langle e_{01}\rangle$, and $\Omega_p = 0$ for $p \geq 2$. The boundary map $\partial e_{01} = e_1 - e_0$ is injective. Hence $H_0 \cong \mathbb{Z}$, and $H_p = 0$ for $p \geq 1$.

Example 2. Consider the directed triangle $i \to j \to k$, $i \to k$. We have:

$$\Omega_0 = \langle i, j, k\rangle, \quad \Omega_1 = \langle e_{ij}, e_{ik}, e_{jk}\rangle, \quad \Omega_2 = \langle e_{ijk}\rangle.$$

$$\ker \partial_1 = \langle e_{ij} + e_{jk} - e_{ik}\rangle.$$

$$\partial_2\, e_{ijk} = e_{jk} - e_{ik} + e_{ij} \ = \ \text{generator of } \ker \partial_1.$$

Thus $H_0 = \mathbb{K}$, $\quad H_1 = 0$, $\quad$ and $\quad H_2 = \ker \partial_2 = 0$.

Example: Directed Square

Example 3. Consider the directed square $G = (V, E)$, with $V = \{0, 1, 2, 3\}$, $E = \{0 \to 1,\ 0 \to 2,\ 1 \to 3,\ 2 \to 3\}$. We have: $\Omega_0 = \mathbb{Z}^4$.
$\mathcal{A}_1 = \mathbb{Z}\langle e_{01}, e_{02}, e_{13}, e_{23}\rangle \cong \mathbb{Z}^4$, and $\Omega_1 = \mathcal{A}_1$ (boundaries are differences of vertices, always in $\mathcal{A}_0$).

Allowed 2**-paths**: $\quad 0 \to 1 \to 3 \ \Rightarrow\ e_{013}, \qquad 0 \to 2 \to 3 \ \Rightarrow\ e_{023}.$

Boundaries: $\quad \partial e_{013} = e_{13} - e_{03} + e_{01}, \qquad \partial e_{023} = e_{23} - e_{03} + e_{02}.$

Since e_{03} is *not* in $\mathcal{A}_1$ (no arc $0 \to 3$), neither e_{013} nor e_{023} lies in Ω_2. However, considering $c = e_{013} - e_{023}$, we have:

$$\partial c = (e_{13} - e_{03} + e_{01}) - (e_{23} - e_{03} + e_{02}) = e_{01} - e_{02} + e_{13} - e_{23} \in \mathcal{A}_1.$$

The e_{03} terms cancel, then $c \in \Omega_2$, and $\Omega_2 = \mathbb{Z}\langle c\rangle \cong \mathbb{Z}$.

Example: Directed Square (cont.)

Also, c is not boundary, since there is no $\alpha \in \Omega_3$ such that $\partial\alpha = c$, given that $\Omega_3 = 0$ (there are no allowed 3-paths). Hence c is a non-trivial cycle.

Path homologies:

$$\begin{aligned} H_0(G;\mathbb{Z}) &\cong \mathbb{Z}, \\ H_1(G;\mathbb{Z}) &= 0 \quad \text{(the boundary map is injective on } \Omega_1\text{)}, \\ H_2(G;\mathbb{Z}) &\cong \mathbb{Z} \quad \text{generated by } [e_{013} - e_{023}], \\ H_p(G;\mathbb{Z}) &= 0 \quad \text{for } p \geq 3. \end{aligned}$$

The class $[e_{013} - e_{023}]$ detects the two-dimensional "hole" formed by the two directed paths from 0 to 3. Note that undirected simplicial homology would see no hole here.

Topological Descriptors: Structure Vectors

Given a path complex $\mathfrak{P}(G)$ associated with a digraph G, we can quantify its topological features using structure vectors:

- **Path structure vector:** $P(\mathfrak{P}) = (p_1, ..., p_n)$, where p_i is the number of i-paths.
- **∂-invariant structure vector:** $V(\mathfrak{P}) = (v_1, ..., v_m)$, where v_i is the number of ∂-invariant i-paths.
- **Betti structure vector:** $B(\mathfrak{P}) = (\beta_0, ..., \beta_k)$, where β_i is the i-th Betti number.
- **Euler structure vector:** $X(\mathfrak{P}) = (\chi_0, ..., \chi_k)$ where χ_i is the i-th Euler characteristic.

PDC for Brain Connectivity Inference

Three Notions of Brain Connectivity

- **Structural (anatomical) connectivity**: Refers to a set of anatomical connections that link neural elements.
- **Functional connectivity**: Refers to the temporal interdependence of activation patterns of anatomically separate brain areas (estimators: correlation, coherence – undirected and symmetric).
- **Effective connectivity**: Reflects the causal relationships between activated brain regions by characterizing the influence that one brain structure has on another (estimators: PDC, DTF – directed and asymmetric.).

Why Partial Directed Coherence?

The Partial Directed Coherence (PDC), proposed by (Baccalá & Sameshima, 2001), was designed to satisfy:

- **Directionality**: For time series $\mathbf{x}_i$ and $\mathbf{x}_j$, distinguish $\mathbf{x}_j \to \mathbf{x}_i$ from $\mathbf{x}_i \to \mathbf{x}_j$.
- **Frequency domain**: Representation of Granger causality in the frequency domain (neural interactions are rhythm-specific).
- **Direct vs. indirect**: Separate $\mathbf{x}_1 \to \mathbf{x}_3$ (direct) from $\mathbf{x}_1 \to \mathbf{x}_2 \to \mathbf{x}_3$ (indirect).
- **Multivariate**: Condition on all other recorded series.

Significance tests and confidence intervals for PDC was introduced latter with the asymptotic theory (Baccalá et al., 2013).

Granger Causality

For two time series $\mathbf{x}(n)$ and $\mathbf{y}(n)$, the series $\mathbf{x}(n)$ Granger-causes $\mathbf{y}(n)$ if the past values of $\mathbf{x}(n)$ contain information that helps to predict $\mathbf{y}(n)$. In other words, let $\mathcal{U}_n$ be all information up to time n and $\mathcal{U}_n \setminus \mathbf{x}(n)$ the same information with the past of $\mathbf{x}(n)$ removed, then:

$$\mathbf{x}(n) \text{ Granger-causes } \mathbf{y}(n) \iff \text{var}\left[\,\mathbf{y}(n) \,|\, \mathcal{U}_{n-1}\,\right] < \text{var}\left[\,\mathbf{y}(n) \,|\, \mathcal{U}_{n-1} \setminus \mathbf{x}(n)\,\right].$$

Granger causality is not reciprocal, i.e. $\mathbf{x}(n)$ Granger-causes $\mathbf{y}(n)$ does not imply that $\mathbf{y}(n)$ Granger-causes $\mathbf{x}(n)$.

The Multivariate Autoregressive (MVAR) Model

Let $\mathbf{x}(n) = [x_1(n), \ldots, x_N(n)]^\mathsf{T}$ be N jointly stationary, zero-mean time series. The MVAR(p) model is

$$\mathbf{x}(n) \;=\; \sum_{r=1}^{p} \mathbf{A}_r\, \mathbf{x}(n-r) \;+\; \mathbf{w}(n), \qquad \mathbf{w}(n) \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma}_\mathbf{w}),$$

with

- $\mathbf{A}_r = [a_{ij}(r)]$ the $N \times N$ coefficient matrix at lag r and $\mathbf{w}(n)$ serially uncorrelated innovations.
- $a_{ij}(r) =$ influence of $x_j(n-r)$ on $x_i(n)$ (row $=$ target, column $=$ source).
- Granger causality $j \not\rightarrow i \iff a_{ij}(r) = 0$ for all $r = 1, \ldots, p$.
- $\boldsymbol{\Sigma}_\mathbf{w}$ is generally **not diagonal**: instantaneous (zero-lag) correlation is absorbed here.

Estimating the MVAR Model

Coefficient estimation methods:

- Ordinary/multivariate least squares
- Yule–Walker (Levinson–Wiggins–Robinson)
- Nuttall–Strand / Vieira–Morf
- ARfit (stepwise least squares, Schneider & Neumaier)

Model order selection (p):

- AIC: $\log\det \hat{\boldsymbol{\Sigma}}_{\mathbf{w}} + \dfrac{2pN^2}{n_s}$
- BIC/SBC: $\log\det \hat{\boldsymbol{\Sigma}}_{\mathbf{w}} + \dfrac{\log(n_s)\, pN^2}{n_s}$
- Hannan–Quinn, FPE

Partial Directed Coherence (PDC) - Going to the Frequency Domain

Define the matrix:

$$\bar{\mathbf{A}}(f) \;=\; \mathbf{I} - \mathbf{A}(f) \;=\; \mathbf{I} - \sum_{r=1}^{p} \mathbf{A}_r \, e^{-i2\pi f r}.$$

Its inverse is the transfer function:

$$\mathbf{H}(f) = \bar{\mathbf{A}}^{-1}(f), \qquad \mathbf{S}(f) = \mathbf{H}(f)\,\boldsymbol{\Sigma}_{\mathbf{w}}\,\mathbf{H}^{\mathrm{H}}(f)$$

where $\mathbf{S}(f)$ is the power spectral density matrix.

Definition. The PDC is defined by (Baccalá & Sameshima, 2001):

$$\pi_{ij}(f) \;=\; \frac{\bar{A}_{ij}(f)}{\sqrt{\bar{\mathbf{a}}_j^{\mathrm{H}}(f)\,\bar{\mathbf{a}}_j(f)}} \;=\; \frac{\bar{A}_{ij}(f)}{\sqrt{\sum_{k=1}^{N} \left|\bar{A}_{kj}(f)\right|^2}}$$

where $\bar{\mathbf{a}}_j(f)$ is the j-th column of $\bar{\mathbf{A}}(f)$.

Properties of PDC

1. **Asymmetric**: $|\pi_{ij}| \neq |\pi_{ji}|$ in general.
2. **Frequency domain**: π_{ij} measures the influence from j to i at frequency f.
3. **Direct**: Indirect paths are excluded by construction.
4. **Normalisation**: $\sum_{i=1}^{N} |\pi_{ij}(f)|^2 = 1$ for every j and every f, and $0 \leq |\pi_{ij}(f)|^2 \leq 1$.
5. **Exact null equivalence**: $\pi_{ij}(f) = 0 \ \forall f \iff a_{ij}(r) = 0 \ \forall r \iff \mathbf{x}_j$ does not Granger-cause $\mathbf{x}_i$ given all other channels.
6. **Multivariate**: Automatically conditioned on the other $N - 2$ series.

Information PDC (iPDC)

The information PDC (iPDC), introduced by (Takahashi et al., 2010a, 2010b), is a modification of the PDC expression that formalizes the relationship between PDC and information flow:

$$\left|\iota\pi_{ij}(f)\right|^2 = \frac{\left|\bar{A}_{ij}(f)\right|^2/\sigma_{ii}}{\bar{\mathbf{a}}_j^{\mathrm{H}}(f)\,\boldsymbol{\Sigma}_{\mathbf{w}}^{-1}\,\bar{\mathbf{a}}_j(f)}.$$

The denominator is a quadratic form in the full inverse innovation covariance $\boldsymbol{\Sigma}_{\mathbf{w}}^{-1}$(off-diagonal terms included).

We can verify that $\iota\pi_{ij}(f)$ is still bounded, $0 \leq |\iota\pi_{ij}(f)|^2 \leq 1$, and still zero exactly when $\mathbf{x}_j \not\to \mathbf{x}_i$.

Also, it reduces to PDC when $\boldsymbol{\Sigma}_{\mathbf{w}} = \sigma^2\mathbf{I}$.

Simulation Studies

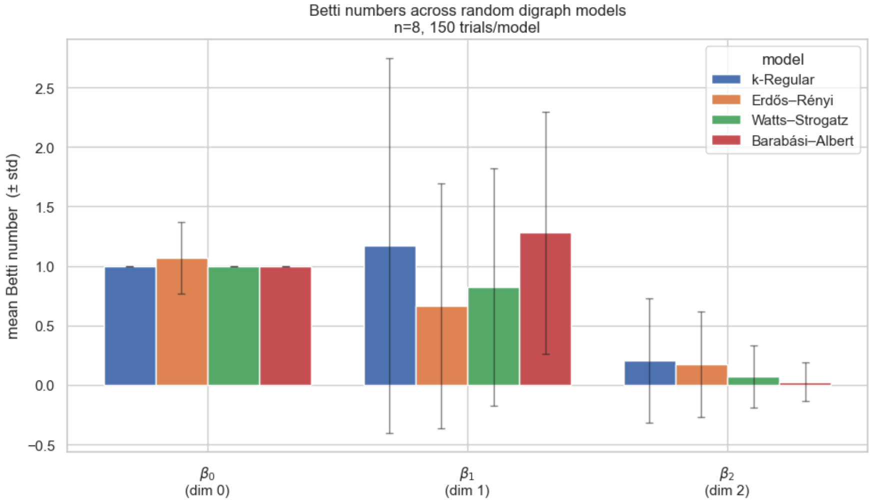
Simulations: Random Digraph Models

We performed simulations on four different random digraph models:

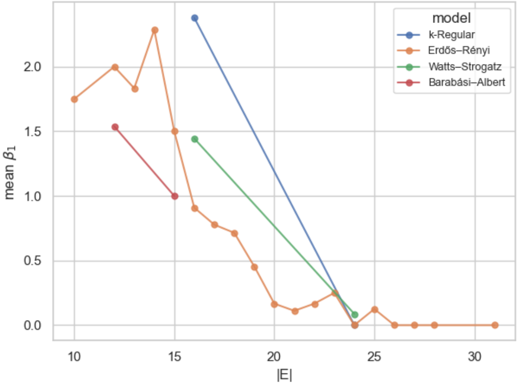
- **k-Regular Random Digraphs**: $R(n, k)$
- **Erdős–Rényi Random Digraphs**: $G(n, p)$
- **Watts-Strogatz Random Digraphs**: $WS(n, N, p)$
- **Barabási-Albert Random Digraphs**: $BA(n, \alpha, \beta, \gamma)$

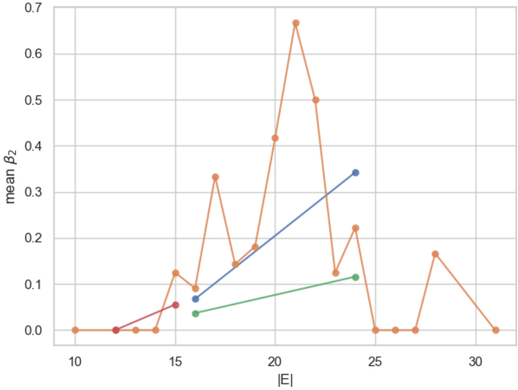
We used digraphs with $n = 8$ vertices and calculated the Betti numbers for 150 trials of each model. The models were implemented in Python using the NetworkX library.

Results: Mean Betti Numbers

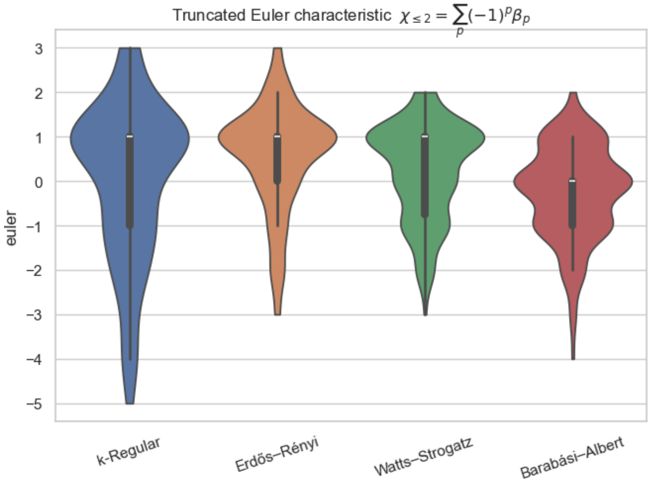


Results: Mean β_1, β_2 vs $|E|$





Results: Euler Characteristic



Applications to Brain Network Analysis

Epilepsy as a Disorder of Brain Connectivity

- Epilepsy is notoriously a brain connectivity network disorder, characterized by a direct relation between **abnormal network dynamics and clinical symptoms**.
- A fact constantly observed in the literature: patients diagnosed with epilepsy present **alterations in brain connectivity networks** in the **ictal phase (seizure)** compared to the **interictal phase**.

EEG Data (Siena Scalp EEG Database)

The EEG data were obtained from the Siena Scalp EEG Database (Detti et al., 2020). We chose eight patients with left temporal lobe epilepsy (TLE) based on the quality of the signal.

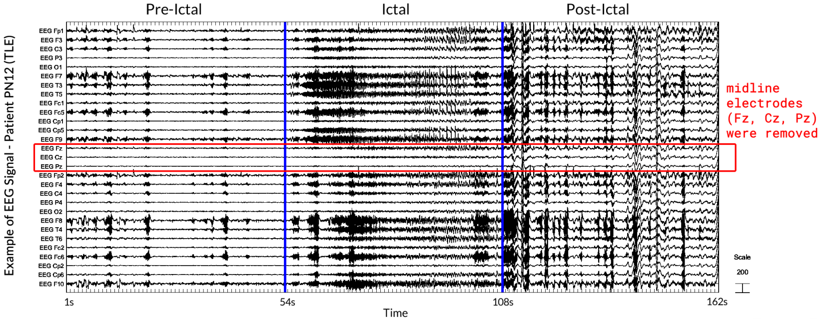
Public available at `https://physionet.org/content/siena-scalp-eeg/1.0.0`.

Table: Patient information.

Pat. id	Age	Gender	Localization	Lateralization	Time (min)
PN01	46	Male	Temporal Lobe	Left	809
PN06	36	Male	Temporal Lobe	Left	722
PN07	20	Female	Temporal Lobe	Left	523
PN09	27	Female	Temporal Lobe	Left	410
PN12	71	Male	Temporal Lobe	Left	246
PN13	34	Female	Temporal Lobe	Left	519
PN14	49	Male	Temporal Lobe	Left	1408
PN16	41	Female	Temporal Lobe	Left	303

Data Preprocessing

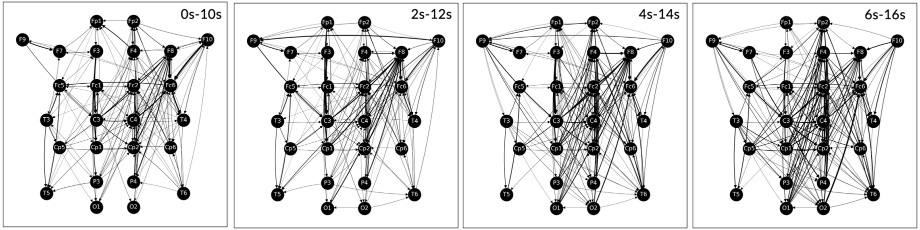
- **1)** Downsampling: from 512 Hz to 256 Hz. **2)** 1 Hz high-pass filter; notch filter at 50 Hz. **3)** The midline electrodes (Fz, Cz, and Pz) were removed (final number of channels: 26). **4)** An ICA was performed to remove artifactual components.
- Next, we identified the **pre-ictal, ictal, and post-ictal phases**, and then divided the signals from each phase into 30s epochs: 30s immediately before the seizures, 30s starting on the seizures onset, and 30s immediately after the seizures.



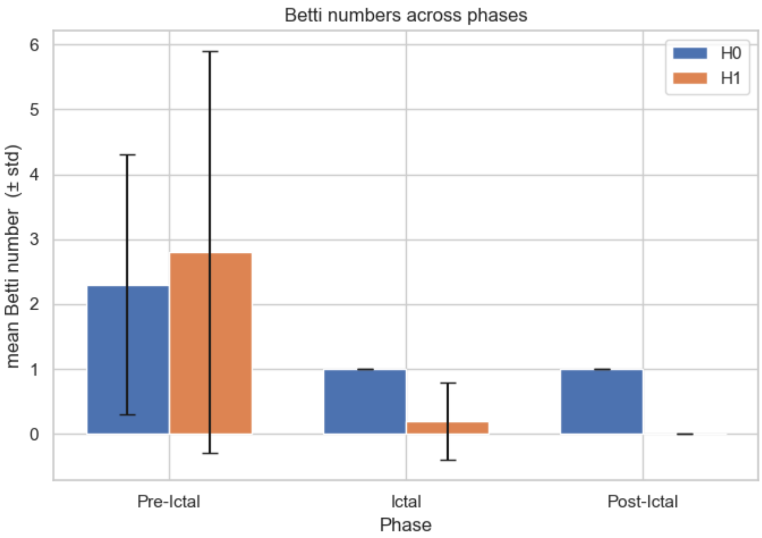
Dynamic iPDC Networks Estimated from the EEG Data

- iPDC $\rightarrow$ **delta** [1 - 4 Hz), **theta** [4 - 8 Hz), and **alpha** [8 - 13 Hz);
- iPDC $\rightarrow$ **Sliding window technique** for each epoch, sliding the window in 10s cuts; overlap of 8s (11 digraphs on each seizure phase).
- VAR autoregression coefficients: estimated through the **Nuttall-Strand's method**. Order for the VAR models: **fixed order $\boldsymbol{p = 12}$**.
- Only the statistically significant connections were considered (estimated asymptotically with a **significance level of 0.1%**). Arc weights were removed.

iPDC networks - Patient PN01 - Delta band [1 Hz, 4Hz) (seizure onset)



Betti Numbers (Path Homologies) – Patient PN01



Thank you!

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